



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 03:51 pm GMT

PDB ID : 9SV8 / pdb_00009sv8
EMDB ID : EMD-55245
Title : Herpes simplex virus 2 delta28-73 glycoprotein C ectodomain in complex with C3b
Authors : Rojas Rechy, M.H.; Atanasiu, D.; Hook, L.M.; Cairns, M.T.; Saw, W.T.; Cahill, A.; Guo, Z.; Calabrese, A.N.; Ranson, N.A.; Friedman, H.M.; Cohen, G.H.; Fontana, J.
Deposited on : 2025-10-02
Resolution : 3.56 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

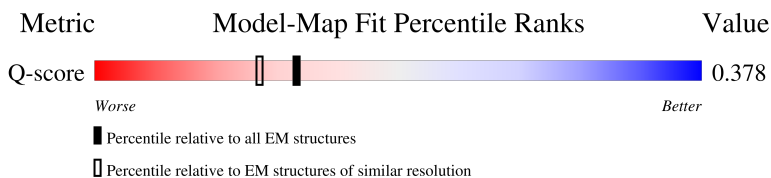
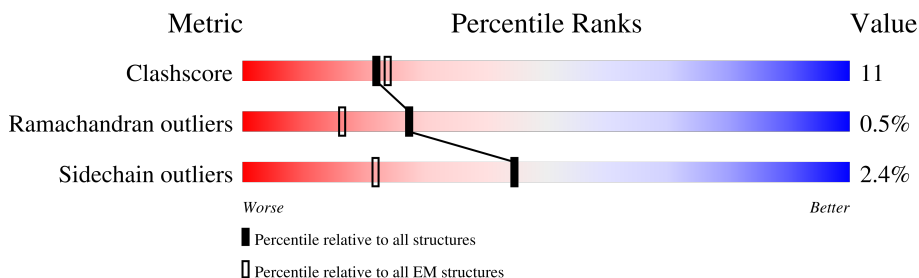
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12750 (3.06 - 4.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	
2	B	645	
3	C	915	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8928 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	166	Total	C	N	O	S	0	0
			1301	809	251	236	5		

- Molecule 2 is a protein called Complement C3 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	628	Total	C	N	O	S	0	0
			4907	3127	830	935	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	LEU	PRO	variant	UNP P01024

- Molecule 3 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	337	Total	C	N	O	S	0	0
			2720	1732	456	516	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	910	GLU	GLN	conflict	UNP P01024

ALA	Y1325	ALA	LEU	MET
CYS	I1326	GLU	GLU	VAL
PRO	S1327	LYS	LYS	VAL
GLY	K1333	HIS	GLY	PHE
VAL	A1334	TYR	TYR	CYS
ASP	F1335	LEU	LEU	PRO
TYR	S1336	MET	TRP	ASN
VAL	D1337	TRP	GLY	
TYR	R1338	GLY	LEU	
LYS		LEU	SER	
THR	V1348	SER	SER	
ARG		ASP	ASP	
LEU	D1353	PHE	TRP	
VAL	D1354	TRP	GLY	
VAL		GLY	GLU	
GLN	H1361	LYS	LYS	
Q1362		PRO	ASN	
	I1368	ASN	ASN	
	I1369	ASP	LEU	
		PHE	SER	
	V1374	ASP	TYR	
		GLU	ILE	
	H1391	TYR	ILE	
	P1392	ILE	ILE	
	E1393	MET	GLY	
		ALA	LYS	
		ILE	ASP	
	G1397	GLU	THR	
		GLN	TRP	
	C1403	THR	VAL	
	R1404	ILE	GLU	
	D1405	LYS	HIS	
		SER	TRP	
	E1406	GLY	PRO	
	L1407	SER	GLU	
	C1408	ASP	GLU	
	R1409	GLU	ASP	
	C1410	VAL	GLU	
		ALA	CYS	
		GLU	GLN	
		GLU	ASP	
		ASN	GLY	
		GLN	GLU	
		CYS	GLU	
		PHE	ASN	
		ILE	GLN	
		THR	LYS	
		GLN	GLN	
		ILE	CYS	
		SER	GLN	
		PRO	ASP	
		ILE	LEU	
		LYS	GLY	
		VAL	ALA	
		THR	PHE	
		LEU	THR	
		GLU	ALA	
		LEU	GLU	
		ARG	LEU	
		ASP	ASP	
		LYS	LYS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	466599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.347	Depositor
Minimum map value	-1.443	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.249	Depositor
Map size (Å)	222.0, 222.0, 222.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/1332	0.74	8/1807 (0.4%)
2	B	0.24	1/5001 (0.0%)	0.51	9/6791 (0.1%)
3	C	0.15	0/2773	0.50	4/3753 (0.1%)
All	All	0.24	1/9106 (0.0%)	0.55	21/12351 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	PRO	CG-CD	-5.72	1.31	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	655	GLU	CA-C-N	13.17	145.41	121.70
3	C	655	GLU	C-N-CA	13.17	145.41	121.70
2	B	56	PRO	CA-N-CD	-12.36	94.69	112.00
2	B	197	SER	CA-C-N	8.38	136.79	121.70
2	B	197	SER	C-N-CA	8.38	136.79	121.70
2	B	56	PRO	N-CD-CG	-8.19	90.91	103.20
3	C	1407	LEU	CA-C-N	-7.64	110.13	120.90
3	C	1407	LEU	C-N-CA	-7.64	110.13	120.90
1	A	263	GLY	N-CA-C	-6.59	104.28	115.08
1	A	195	ARG	CA-C-N	-6.25	111.91	122.92
1	A	195	ARG	C-N-CA	-6.25	111.91	122.92
2	B	361	PRO	CA-N-CD	-5.94	103.69	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLY	N-CA-C	-5.89	106.89	113.79
1	A	336	ALA	N-CA-C	5.85	117.54	109.29
2	B	149	GLU	N-CA-C	-5.62	106.39	113.18
1	A	191	GLY	O-C-N	-5.22	116.55	121.77
1	A	230	VAL	CA-C-N	-5.21	114.49	122.87
1	A	230	VAL	C-N-CA	-5.21	114.49	122.87
2	B	148	PRO	O-C-N	5.11	129.09	122.24
2	B	393	PRO	CA-C-N	-5.03	112.95	121.85
2	B	393	PRO	C-N-CA	-5.03	112.95	121.85

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	GLY	Mainchain
1	A	195	ARG	Sidechain
1	A	229	ARG	Sidechain
1	A	304	ALA	Mainchain
1	A	341	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1301	0	1263	66	0
2	B	4907	0	4974	90	0
3	C	2720	0	2720	63	0
All	All	8928	0	8957	202	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:CD1	1:A:341:ARG:CD	1.76	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:CD1	1:A:341:ARG:HD3	1.02	1.47
1:A:339:LEU:HD13	1:A:341:ARG:CG	1.52	1.35
1:A:339:LEU:HD11	1:A:341:ARG:CD	1.43	1.34
1:A:339:LEU:HD13	1:A:341:ARG:CD	1.47	1.27
1:A:270:TRP:HH2	1:A:299:THR:C	1.45	1.23
1:A:339:LEU:HD13	1:A:341:ARG:HG2	1.19	1.11
1:A:339:LEU:CD1	1:A:341:ARG:CG	2.19	1.10
1:A:339:LEU:CG	1:A:341:ARG:HD3	1.83	1.08
1:A:270:TRP:CH2	1:A:300:VAL:N	2.20	1.06
1:A:338:VAL:HG23	1:A:340:PRO:HD3	1.39	1.01
1:A:270:TRP:CH2	1:A:299:THR:C	2.37	1.01
1:A:339:LEU:HD11	1:A:341:ARG:NE	1.80	0.95
1:A:339:LEU:CD1	1:A:341:ARG:HG2	1.94	0.91
1:A:304:ALA:C	1:A:306:GLY:H	1.76	0.91
1:A:339:LEU:HD11	1:A:341:ARG:HD3	0.93	0.91
3:C:706:MET:HG3	3:C:712:ILE:HG22	1.57	0.87
1:A:338:VAL:CG2	1:A:340:PRO:HD3	2.05	0.85
1:A:210:MET:HA	1:A:229:ARG:HA	1.60	0.83
2:B:373:ASP:C	2:B:375:VAL:H	1.87	0.82
1:A:96:CYS:HA	1:A:113:CYS:HB3	1.62	0.82
1:A:339:LEU:CD2	1:A:341:ARG:HD3	2.09	0.82
1:A:241:HIS:CD2	1:A:243:HIS:CD2	2.70	0.80
1:A:241:HIS:CD2	1:A:243:HIS:NE2	2.49	0.80
1:A:270:TRP:HH2	1:A:300:VAL:N	1.54	0.80
1:A:241:HIS:HD2	1:A:243:HIS:NE2	1.81	0.79
1:A:304:ALA:C	1:A:306:GLY:N	2.41	0.78
1:A:270:TRP:HH2	1:A:299:THR:O	1.70	0.72
1:A:339:LEU:HD13	1:A:341:ARG:HD3	1.12	0.72
3:C:655:GLU:H	3:C:656:GLU:HB2	1.56	0.71
1:A:211:TYR:HB2	1:A:228:VAL:HB	1.73	0.70
2:B:372:GLU:CD	2:B:373:ASP:OD2	2.35	0.70
3:C:654:ALA:HB3	3:C:657:ASN:HB2	1.73	0.70
1:A:307:GLY:O	1:A:309:GLY:N	2.24	0.70
2:B:373:ASP:C	2:B:375:VAL:N	2.50	0.69
1:A:194:GLY:HA3	1:A:195:ARG:HH21	1.57	0.69
1:A:98:ARG:HB2	1:A:101:PRO:HG3	1.75	0.69
1:A:338:VAL:HG23	1:A:340:PRO:CD	2.18	0.67
2:B:147:ASN:HB2	2:B:151:ILE:HG13	1.76	0.66
2:B:179:MET:HA	2:B:179:MET:HE3	1.79	0.65
2:B:114:LYS:NZ	3:C:666:GLU:OE1	2.30	0.65
2:B:116:ILE:HG22	2:B:580:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ASP:OD1	2:B:117:TYR:OH	2.17	0.63
2:B:343:LYS:HB2	2:B:346:MET:HG3	1.81	0.63
3:C:1404:ARG:O	3:C:1405:ASP:C	2.42	0.62
3:C:820:ASP:OD1	3:C:821:GLY:N	2.33	0.62
3:C:1302:ILE:HG12	3:C:1374:VAL:HG22	1.83	0.59
1:A:191:GLY:O	1:A:196:GLN:NE2	2.34	0.59
1:A:270:TRP:CH2	1:A:299:THR:O	2.51	0.59
1:A:237:SER:H	1:A:258:ALA:HB3	1.66	0.59
3:C:753:GLN:OE1	3:C:753:GLN:N	2.31	0.58
1:A:323:ASP:OD1	1:A:323:ASP:N	2.37	0.57
2:B:175:GLU:OE2	3:C:827:LYS:NZ	2.29	0.57
3:C:1296:THR:OG1	3:C:1297:MET:N	2.37	0.57
2:B:111:GLN:OE1	2:B:126:ARG:NH1	2.37	0.57
3:C:739:ASN:ND2	3:C:831:GLU:OE2	2.38	0.57
1:A:211:TYR:O	1:A:228:VAL:N	2.37	0.57
2:B:46:VAL:O	2:B:47:LEU:C	2.46	0.56
3:C:1294:ASP:N	3:C:1294:ASP:OD1	2.38	0.56
2:B:457:MET:HE1	2:B:462:GLU:HA	1.86	0.56
2:B:465:ILE:HD11	2:B:515:LEU:HD13	1.88	0.56
3:C:732:LEU:HD23	3:C:826:LEU:HB2	1.87	0.55
3:C:1407:LEU:O	3:C:1408:CYS:C	2.47	0.55
2:B:381:GLY:C	2:B:383:GLY:H	2.15	0.55
2:B:542:VAL:HB	2:B:564:GLU:HB3	1.88	0.55
2:B:335:PHE:HE1	2:B:352:VAL:HG22	1.72	0.55
2:B:2:PRO:HB3	2:B:27:ALA:HB2	1.88	0.55
1:A:260:TYR:HE1	1:A:266:ALA:HB2	1.72	0.55
2:B:148:PRO:HD3	2:B:182:TRP:CD1	2.41	0.55
1:A:192:PRO:HD2	1:A:195:ARG:HD2	1.90	0.54
2:B:205:TYR:OH	3:C:666:GLU:OE1	2.22	0.54
2:B:268:ARG:HH21	3:C:1297:MET:HE3	1.73	0.54
3:C:661:ARG:HB3	3:C:694:ASP:HB3	1.89	0.54
3:C:1404:ARG:O	3:C:1406:GLU:N	2.41	0.53
2:B:249:VAL:HG11	2:B:278:VAL:HG21	1.90	0.53
3:C:816:HIS:HB3	3:C:818:ILE:HG12	1.91	0.53
2:B:500:THR:H	2:B:503:PHE:HD1	1.57	0.52
1:A:339:LEU:CD2	1:A:341:ARG:CD	2.83	0.52
2:B:588:LYS:NZ	3:C:700:GLU:OE2	2.43	0.52
1:A:234:ARG:HD3	1:A:259:THR:HG21	1.91	0.51
1:A:235:PRO:HA	1:A:320:TRP:CZ3	2.45	0.51
2:B:350:LEU:HD11	2:B:400:ILE:HD13	1.93	0.51
2:B:372:GLU:CD	2:B:373:ASP:CG	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:827:LYS:HE2	3:C:829:VAL:HG12	1.92	0.51
2:B:197:SER:HB3	2:B:198:THR:HA	1.93	0.50
2:B:7:ILE:HG23	2:B:622:LEU:HD21	1.93	0.50
2:B:89:THR:HG23	2:B:94:VAL:HG22	1.93	0.50
2:B:126:ARG:CZ	2:B:572:VAL:HB	2.42	0.50
2:B:373:ASP:O	2:B:375:VAL:N	2.45	0.49
2:B:105:SER:HB3	2:B:139:ARG:HH22	1.75	0.49
2:B:430:SER:OG	2:B:523:GLU:OE2	2.27	0.49
3:C:665:PRO:HG3	3:C:693:LYS:HE3	1.94	0.49
2:B:25:HIS:NE2	2:B:512:TYR:OH	2.43	0.49
2:B:428:GLY:O	2:B:429:ASN:C	2.56	0.49
3:C:814:TYR:HB3	3:C:815:HIS:ND1	2.28	0.49
2:B:372:GLU:OE2	2:B:373:ASP:OD2	2.29	0.49
2:B:12:LEU:HB2	2:B:101:VAL:HG22	1.95	0.48
1:A:339:LEU:HD11	1:A:341:ARG:HE	1.69	0.48
1:A:329:ARG:NH1	3:C:1286:CYS:SG	2.86	0.48
2:B:322:SER:OG	2:B:323:GLY:N	2.47	0.48
1:A:192:PRO:HD2	1:A:195:ARG:CD	2.44	0.48
2:B:594:ILE:HG21	3:C:712:ILE:HD11	1.96	0.48
2:B:126:ARG:NH2	2:B:573:LEU:O	2.28	0.48
2:B:210:PHE:HA	2:B:237:PHE:HA	1.96	0.48
2:B:219:LYS:HA	2:B:219:LYS:HD3	1.70	0.48
2:B:442:GLU:OE2	2:B:444:ARG:NE	2.46	0.48
1:A:194:GLY:C	1:A:195:ARG:HG3	2.38	0.48
1:A:325:VAL:HG11	3:C:1318:LEU:HG	1.95	0.48
2:B:342:PHE:O	2:B:424:TYR:N	2.46	0.48
2:B:8:THR:HG22	2:B:20:MET:HG2	1.95	0.47
3:C:772:LEU:HD13	3:C:1368:LEU:HD13	1.96	0.47
2:B:410:SER:N	2:B:413:GLU:OE1	2.38	0.47
3:C:1311:ASP:OD2	3:C:1361:HIS:NE2	2.39	0.47
2:B:434:LEU:HB2	2:B:513:TYR:HE2	1.79	0.47
2:B:453:PHE:HB2	2:B:493:VAL:HB	1.97	0.47
2:B:10:ASN:HD22	2:B:635:ARG:HH11	1.62	0.47
2:B:541:LEU:HD21	3:C:705:SER:HB3	1.97	0.47
3:C:1391:HIS:CD2	3:C:1392:PRO:HD2	2.49	0.47
3:C:1404:ARG:O	3:C:1407:LEU:HG	2.14	0.47
1:A:98:ARG:NH1	3:C:1321:GLY:O	2.48	0.47
1:A:265:ARG:HG2	1:A:266:ALA:N	2.29	0.47
3:C:1295:ALA:HB3	3:C:1348:VAL:HG22	1.96	0.47
3:C:1315:LEU:HA	3:C:1318:LEU:HD12	1.96	0.46
2:B:73:GLU:H	2:B:73:GLU:HG3	1.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LEU:HD22	2:B:33:VAL:HG11	1.98	0.46
2:B:335:PHE:HD1	2:B:338:THR:HG21	1.79	0.46
2:B:179:MET:HE2	2:B:203:LYS:HA	1.98	0.46
2:B:108:LEU:HB2	2:B:196:PHE:HD1	1.81	0.46
3:C:817:PHE:C	3:C:818:ILE:HD13	2.41	0.46
1:A:304:ALA:O	1:A:306:GLY:N	2.49	0.46
1:A:341:ARG:HA	1:A:341:ARG:HD2	1.67	0.46
2:B:325:PRO:HG2	2:B:357:PRO:HB2	1.97	0.46
2:B:524:VAL:HG23	2:B:630:GLN:NE2	2.31	0.45
2:B:528:SER:OG	2:B:609:SER:N	2.49	0.45
1:A:114:ARG:NH1	1:A:195:ARG:HB3	2.30	0.45
1:A:192:PRO:O	1:A:193:LEU:C	2.59	0.45
2:B:13:ARG:HH22	2:B:477:ARG:HB3	1.82	0.45
2:B:458:ASP:N	2:B:458:ASP:OD1	2.48	0.45
3:C:1289:TYR:CD1	3:C:1295:ALA:HB2	2.51	0.45
1:A:307:GLY:C	1:A:309:GLY:N	2.74	0.45
2:B:392:HIS:O	2:B:394:SER:N	2.50	0.45
2:B:24:ALA:HB3	2:B:60:HIS:HB3	1.97	0.45
3:C:736:VAL:HG22	3:C:826:LEU:HD11	1.98	0.45
2:B:148:PRO:HD3	2:B:182:TRP:NE1	2.32	0.45
1:A:204:THR:H	1:A:207:THR:HG1	1.63	0.44
2:B:541:LEU:HD12	3:C:713:CYS:SG	2.57	0.44
1:A:323:ASP:OD1	1:A:326:SER:OG	2.32	0.44
2:B:221:TYR:HD2	2:B:326:ILE:HG12	1.82	0.44
2:B:571:VAL:HG12	3:C:705:SER:HB3	1.99	0.44
3:C:1335:PHE:HA	3:C:1338:ARG:CZ	2.48	0.44
3:C:770:CYS:HB2	3:C:800:LEU:HD11	2.00	0.44
1:A:260:TYR:HB3	1:A:294:PHE:HB2	2.00	0.44
1:A:103:ALA:HB3	1:A:203:LEU:HD23	1.99	0.43
3:C:783:VAL:HB	3:C:791:LEU:HD21	1.99	0.43
3:C:1325:TYR:CE1	3:C:1327:SER:HA	2.52	0.43
2:B:3:MET:HE1	2:B:514:THR:HG21	1.99	0.43
2:B:63:ASN:OD1	2:B:63:ASN:N	2.52	0.43
3:C:1391:HIS:HB2	3:C:1397:GLY:HA2	2.00	0.43
2:B:110:ILE:HG12	2:B:127:ILE:HG12	1.99	0.43
2:B:114:LYS:HG2	2:B:576:VAL:HG13	2.01	0.43
2:B:373:ASP:HB2	2:B:375:VAL:HG23	1.93	0.43
3:C:1251:ASP:N	3:C:1251:ASP:OD1	2.50	0.43
3:C:1335:PHE:HA	3:C:1338:ARG:NH2	2.33	0.43
3:C:1333:LYS:NZ	3:C:1337:ASP:HB2	2.33	0.43
2:B:111:GLN:HE21	3:C:702:LEU:HD23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:CYS:HA	1:A:113:CYS:CB	2.40	0.43
2:B:1:SER:HA	2:B:2:PRO:HD3	1.87	0.43
2:B:578:LYS:HB3	2:B:578:LYS:HE3	1.84	0.42
3:C:658:ILE:HG21	3:C:810:LYS:HG3	2.00	0.42
3:C:1404:ARG:C	3:C:1406:GLU:N	2.76	0.42
2:B:381:GLY:C	2:B:383:GLY:N	2.75	0.42
2:B:584:ASN:OD1	2:B:586:LYS:HG2	2.19	0.42
2:B:239:TYR:HB2	3:C:723:MET:HE1	2.01	0.42
3:C:738:ARG:NH2	3:C:1406:GLU:HB3	2.34	0.42
1:A:307:GLY:O	1:A:308:GLN:C	2.62	0.42
1:A:329:ARG:HB2	3:C:1353:ASP:HB2	2.01	0.42
1:A:270:TRP:CE3	1:A:283:ILE:HG22	2.55	0.42
1:A:273:ASP:HA	1:A:313:THR:HG22	2.01	0.41
2:B:80:ARG:HA	2:B:80:ARG:HD3	1.65	0.41
2:B:34:THR:HG23	2:B:51:LYS:HG2	2.01	0.41
3:C:1369:ILE:O	3:C:1369:ILE:HG13	2.19	0.41
2:B:474:ASN:ND2	2:B:503:PHE:HA	2.34	0.41
3:C:708:ASP:OD1	3:C:708:ASP:N	2.54	0.41
2:B:260:ILE:O	2:B:260:ILE:HG13	2.20	0.41
2:B:380:GLN:O	2:B:381:GLY:C	2.62	0.41
3:C:697:THR:O	3:C:722:VAL:HG12	2.21	0.41
1:A:327:PHE:HE1	1:A:329:ARG:HE	1.69	0.41
2:B:512:TYR:HD2	2:B:524:VAL:HG13	1.86	0.41
2:B:571:VAL:HG23	3:C:673:GLU:HB3	2.02	0.41
3:C:802:THR:O	3:C:805:GLN:NE2	2.53	0.41
3:C:1354:ASP:OD1	3:C:1354:ASP:O	2.39	0.41
1:A:284:HIS:O	1:A:298:SER:OG	2.28	0.41
2:B:107:TYR:HA	2:B:196:PHE:HE1	1.85	0.41
2:B:346:MET:HB3	2:B:346:MET:HE3	1.80	0.41
3:C:1362:GLN:O	3:C:1362:GLN:HG3	2.21	0.41
2:B:239:TYR:HB2	3:C:723:MET:SD	2.61	0.40
3:C:655:GLU:N	3:C:656:GLU:HB2	2.30	0.40
3:C:698:THR:OG1	3:C:721:THR:HG22	2.21	0.40
1:A:264:ASN:HD22	1:A:264:ASN:N	2.19	0.40
2:B:7:ILE:HD13	2:B:471:LEU:HD11	2.04	0.40
2:B:148:PRO:HD3	2:B:182:TRP:HE1	1.87	0.40
2:B:179:MET:HE1	2:B:202:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/479 (33%)	135 (86%)	19 (12%)	2 (1%)	10	42
2	B	618/645 (96%)	602 (97%)	13 (2%)	3 (0%)	25	59
3	C	331/915 (36%)	320 (97%)	10 (3%)	1 (0%)	37	67
All	All	1105/2039 (54%)	1057 (96%)	42 (4%)	6 (0%)	27	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
3	C	1405	ASP
2	B	374	THR
1	A	305	VAL
2	B	44	LYS
2	B	382	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/390 (36%)	131 (94%)	9 (6%)	14	42
2	B	556/567 (98%)	544 (98%)	12 (2%)	47	70
3	C	310/810 (38%)	307 (99%)	3 (1%)	73	85
All	All	1006/1767 (57%)	982 (98%)	24 (2%)	45	68

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	193	LEU
1	A	195	ARG
1	A	264	ASN
1	A	305	VAL
1	A	323	ASP
1	A	338	VAL
1	A	339	LEU
1	A	341	ARG
2	B	44	LYS
2	B	45	LEU
2	B	46	VAL
2	B	73	GLU
2	B	151	ILE
2	B	214	VAL
2	B	293	ARG
2	B	346	MET
2	B	373	ASP
2	B	382	ASP
2	B	479	LEU
2	B	630	GLN
3	C	1393	GLU
3	C	1405	ASP
3	C	1407	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	264	ASN
2	B	190	ASN
2	B	356	ASN
2	B	630	GLN
3	C	816	HIS
3	C	1362	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

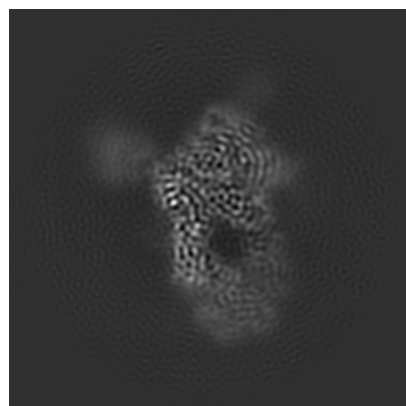
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55245. These allow visual inspection of the internal detail of the map and identification of artifacts.

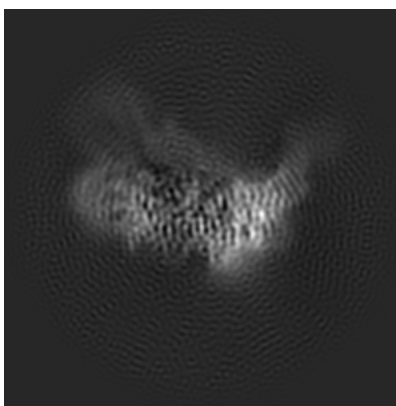
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

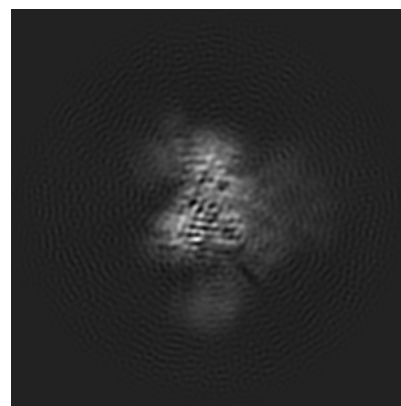
6.1.1 Primary map



X

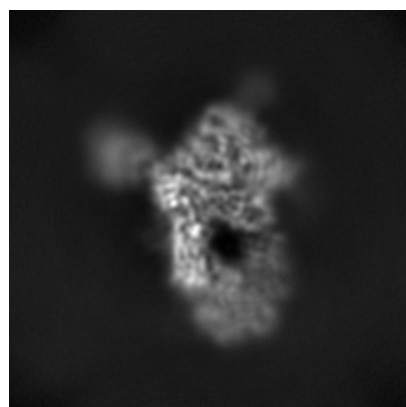


Y

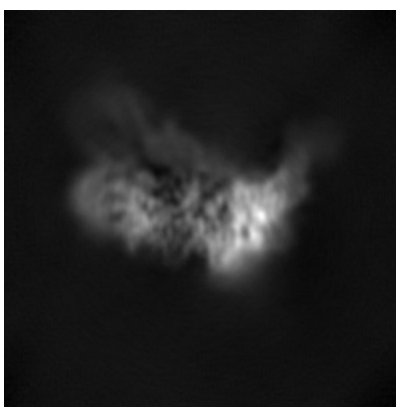


Z

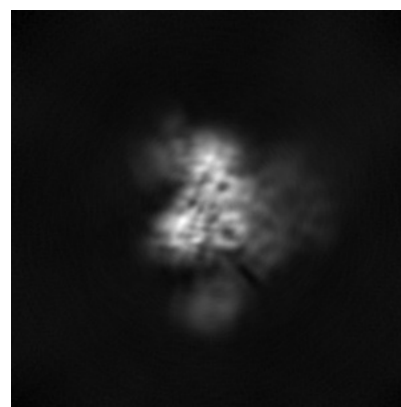
6.1.2 Raw map



X



Y

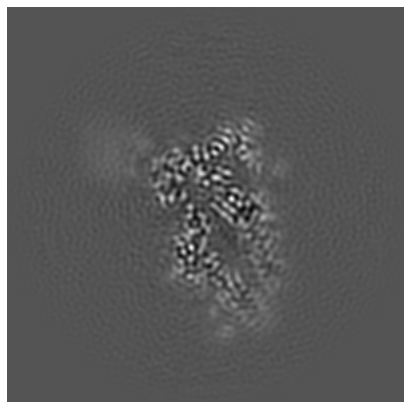


Z

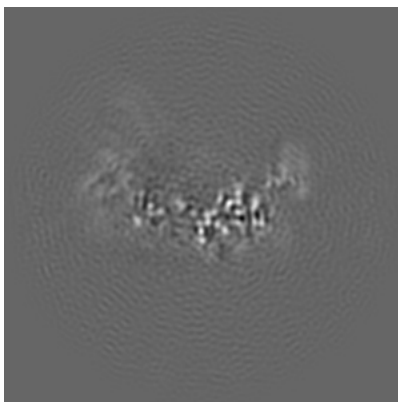
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

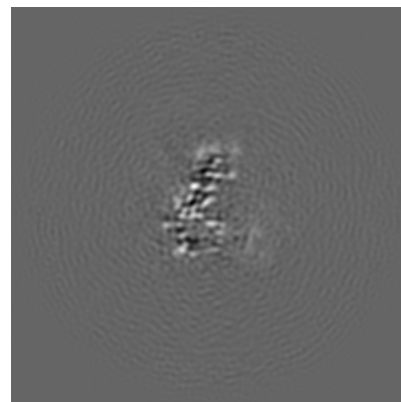
6.2.1 Primary map



X Index: 150

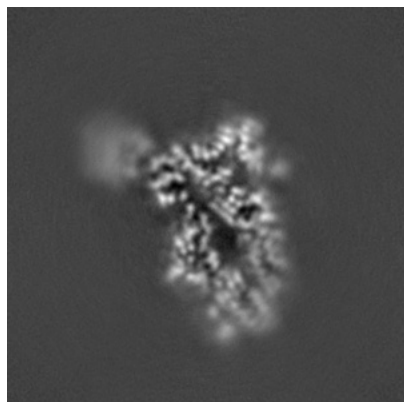


Y Index: 150

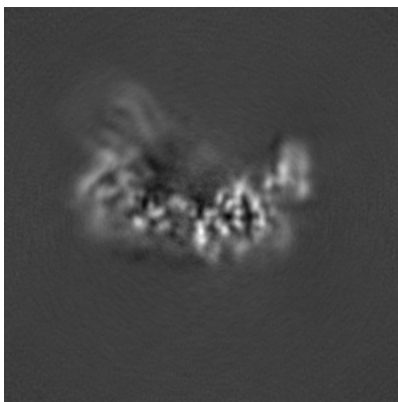


Z Index: 150

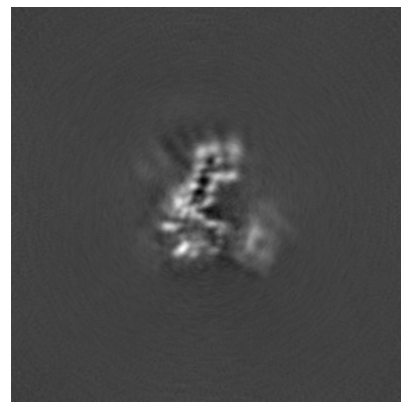
6.2.2 Raw map



X Index: 150



Y Index: 150

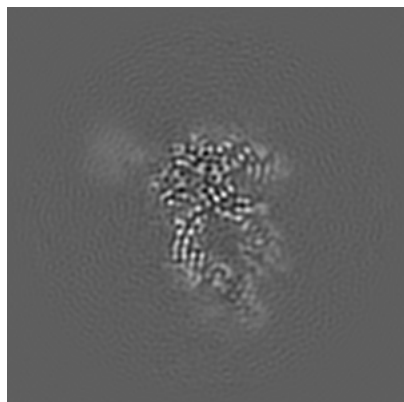


Z Index: 150

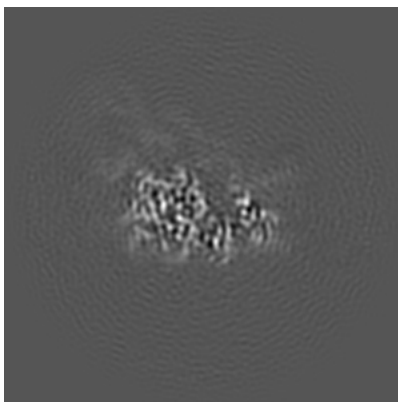
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

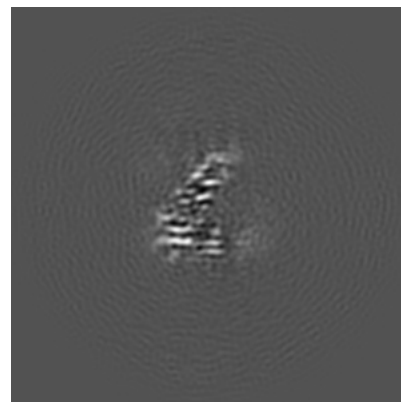
6.3.1 Primary map



X Index: 142

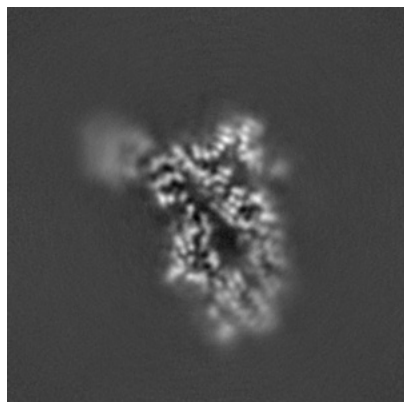


Y Index: 138

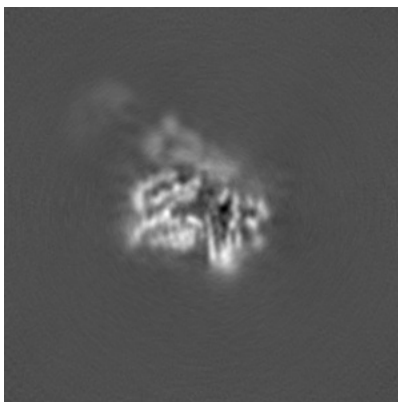


Z Index: 155

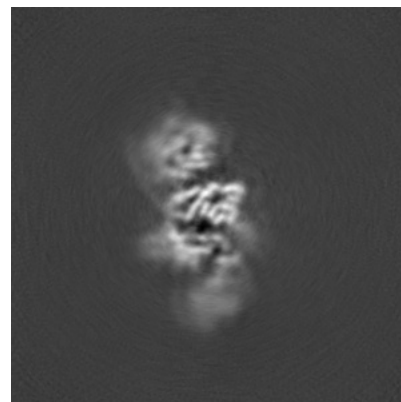
6.3.2 Raw map



X Index: 151



Y Index: 126

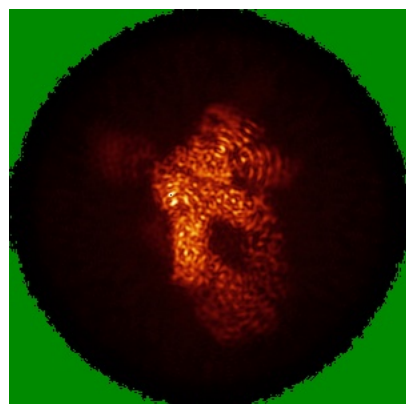


Z Index: 175

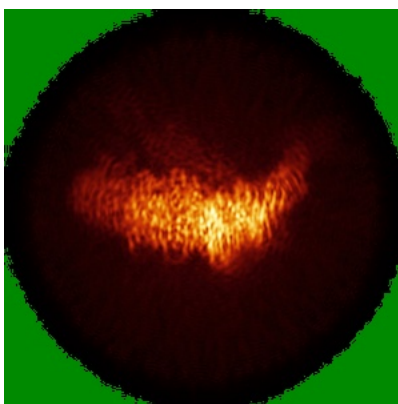
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

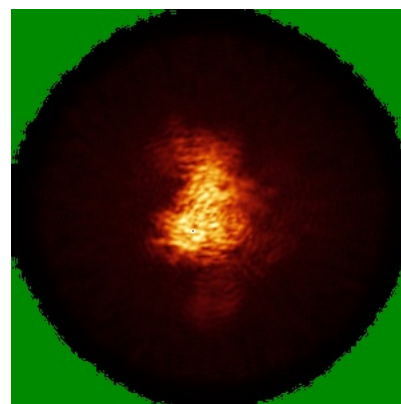
6.4.1 Primary map



X

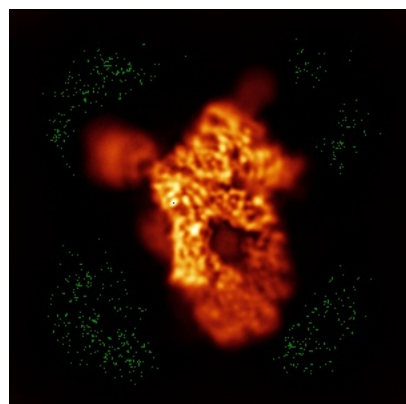


Y

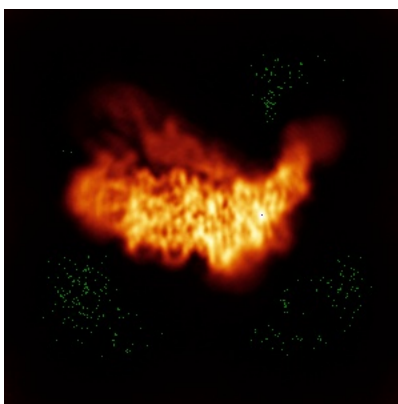


Z

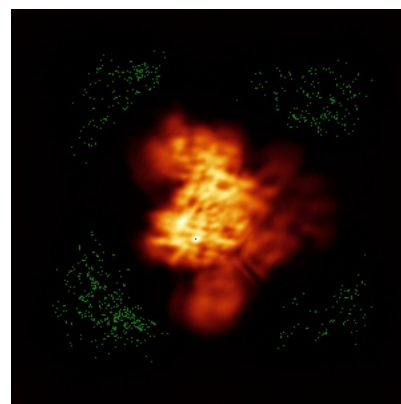
6.4.2 Raw map



X



Y

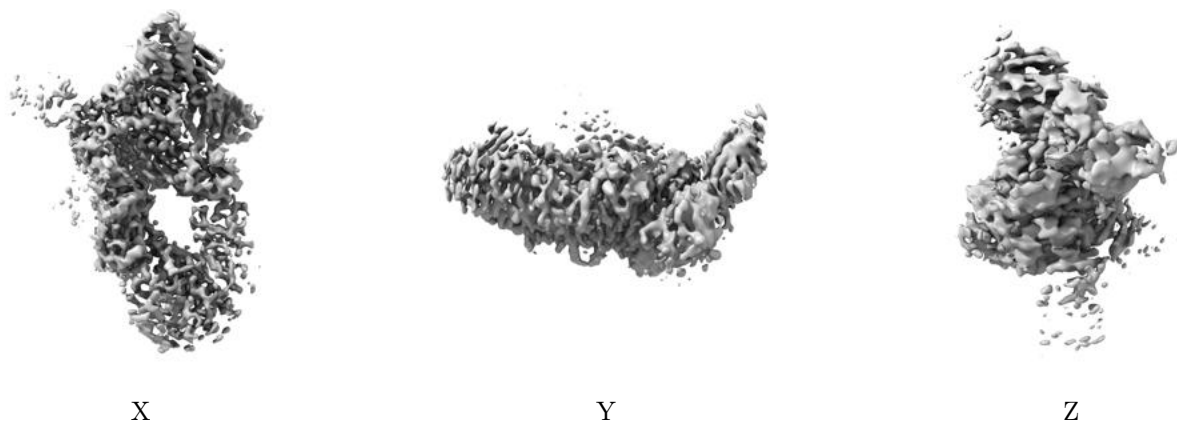


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

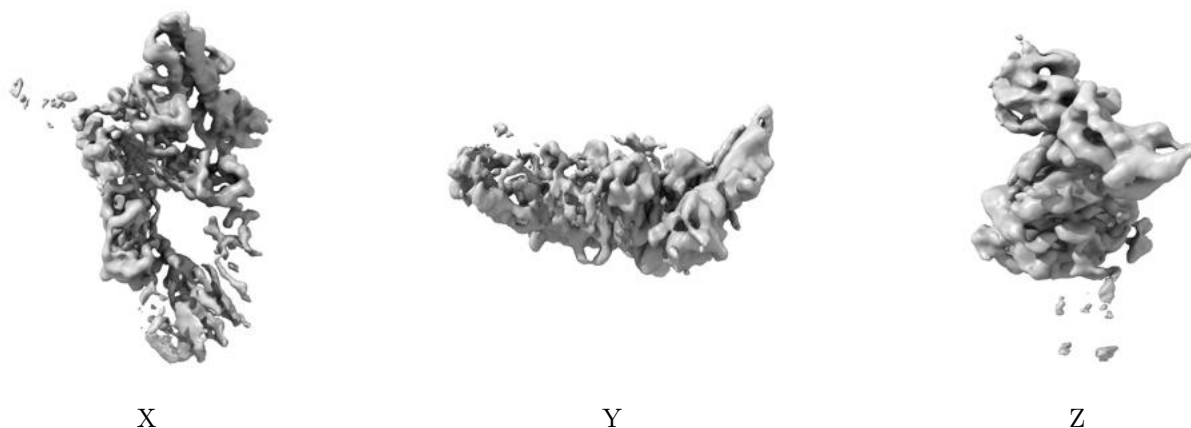
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.249. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

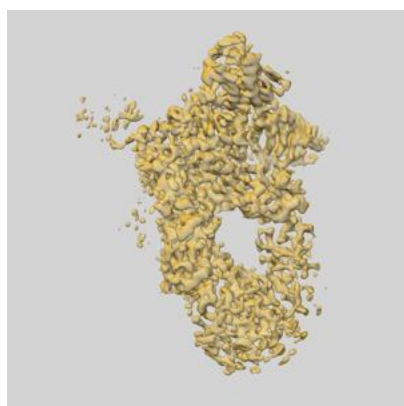
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

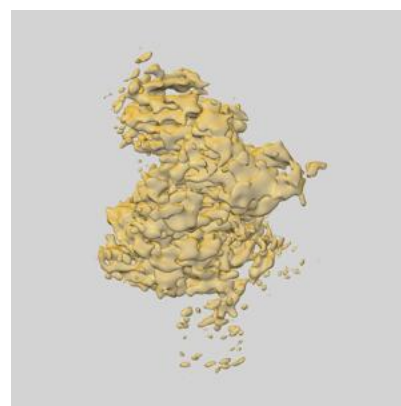
6.6.1 emd_55245_msk_1.map [i](#)



X



Y

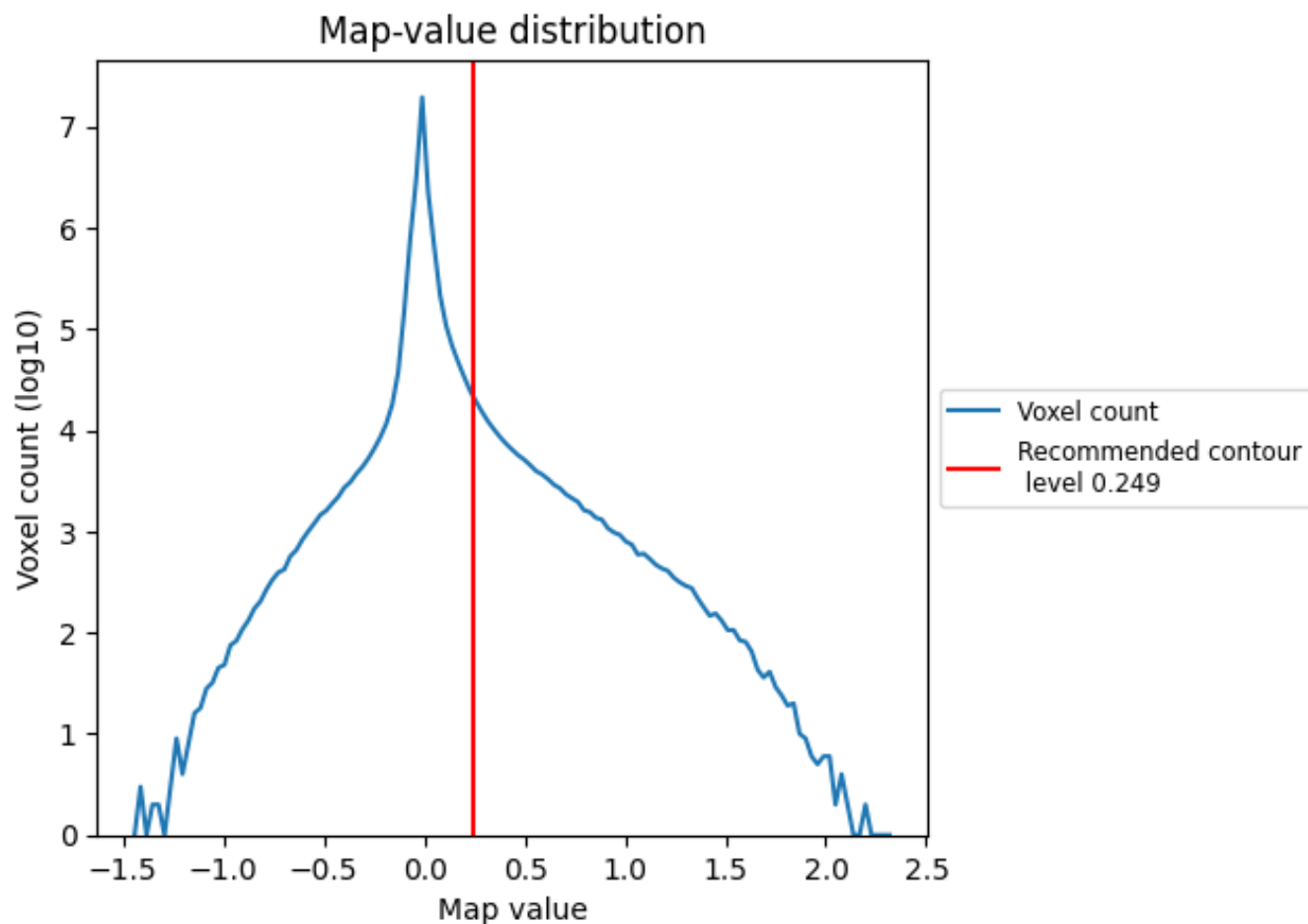


Z

7 Map analysis [i](#)

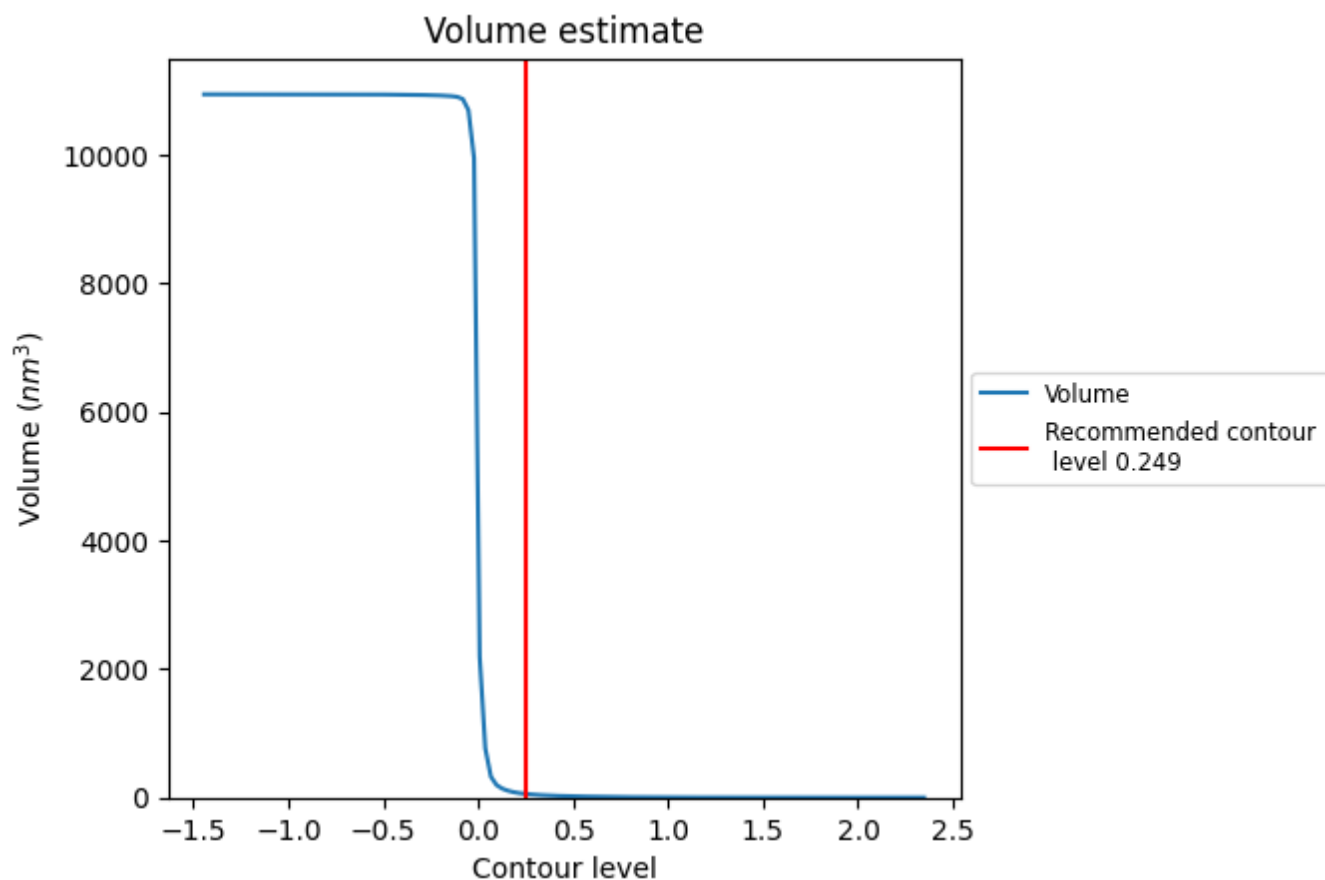
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

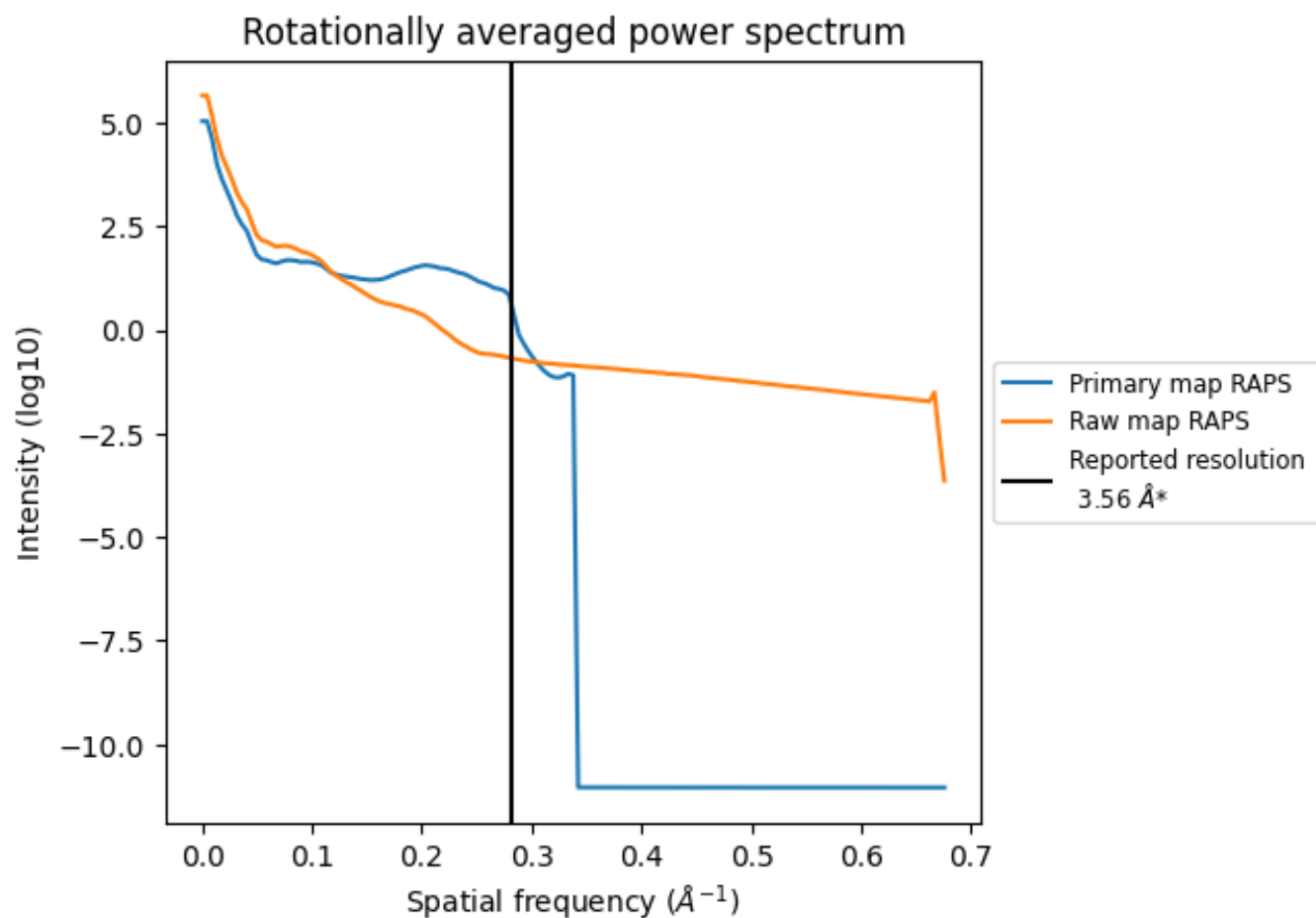
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm^3 ; this corresponds to an approximate mass of 51 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

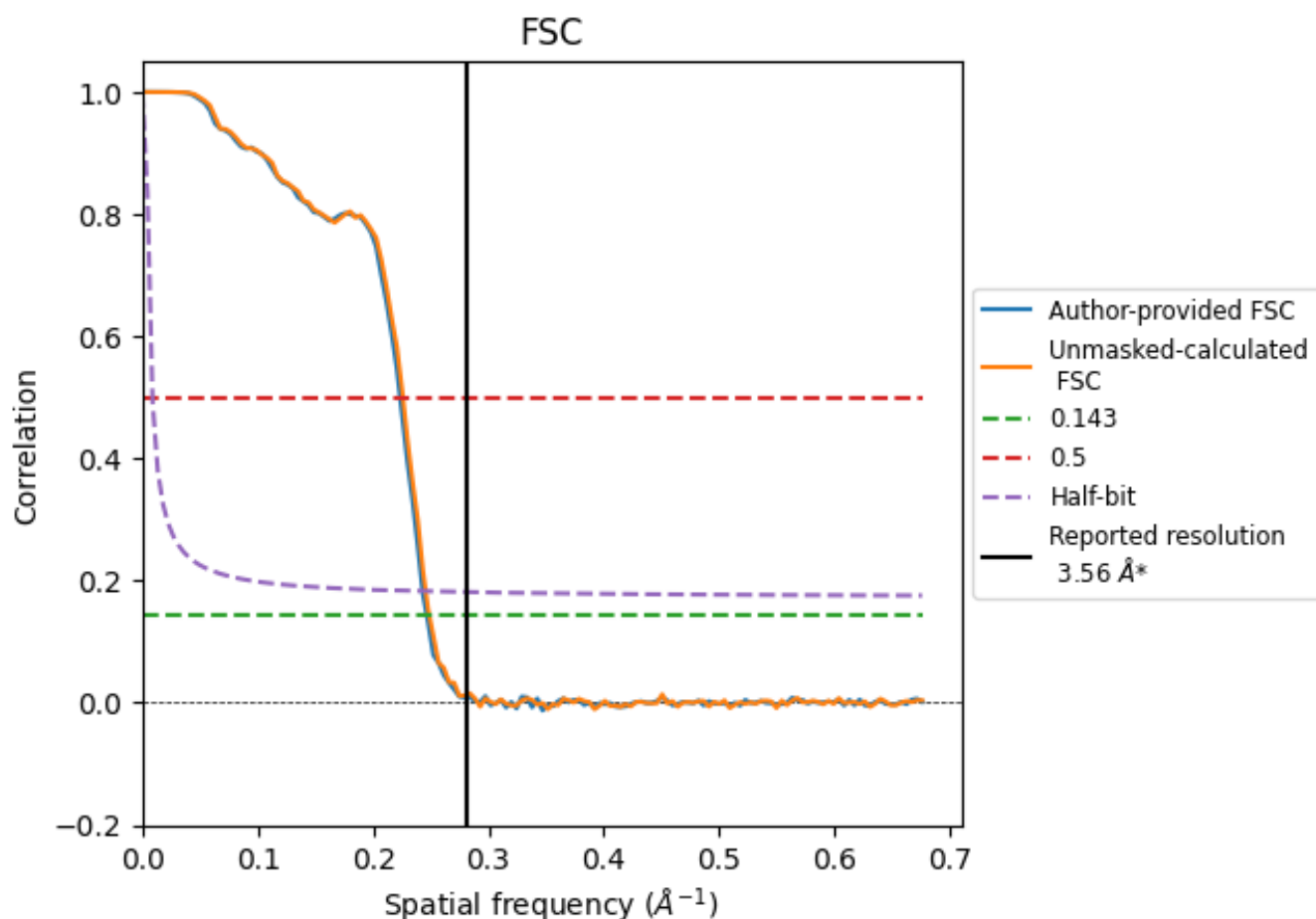


*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.281 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	4.06	4.48	4.12
Unmasked-calculated*	4.02	4.43	4.07

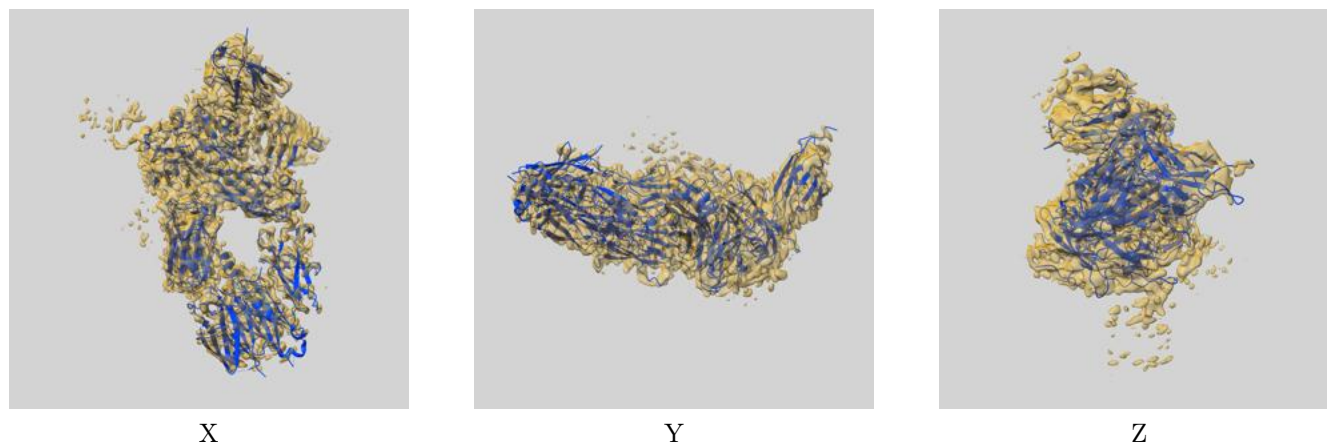
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.56 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.56 by more than 10 %

9 Map-model fit [i](#)

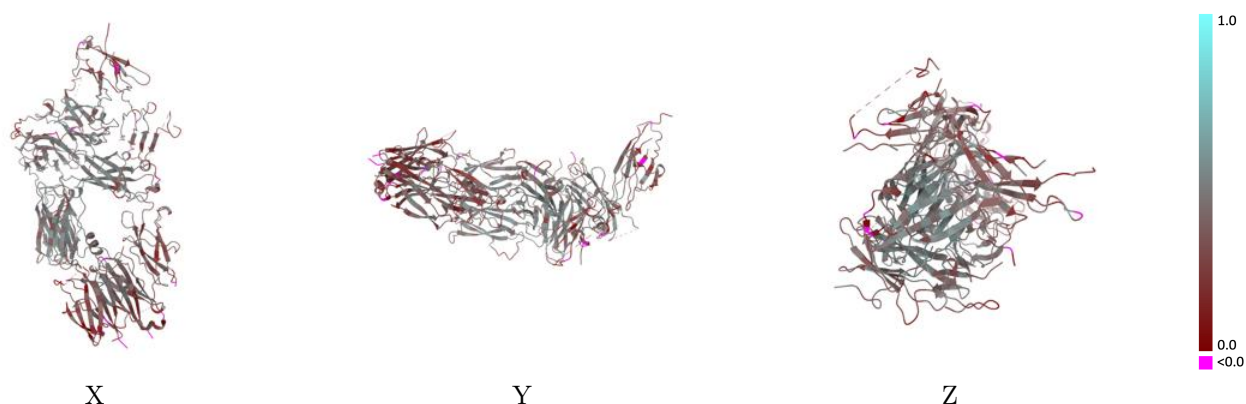
This section contains information regarding the fit between EMDB map EMD-55245 and PDB model 9SV8. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



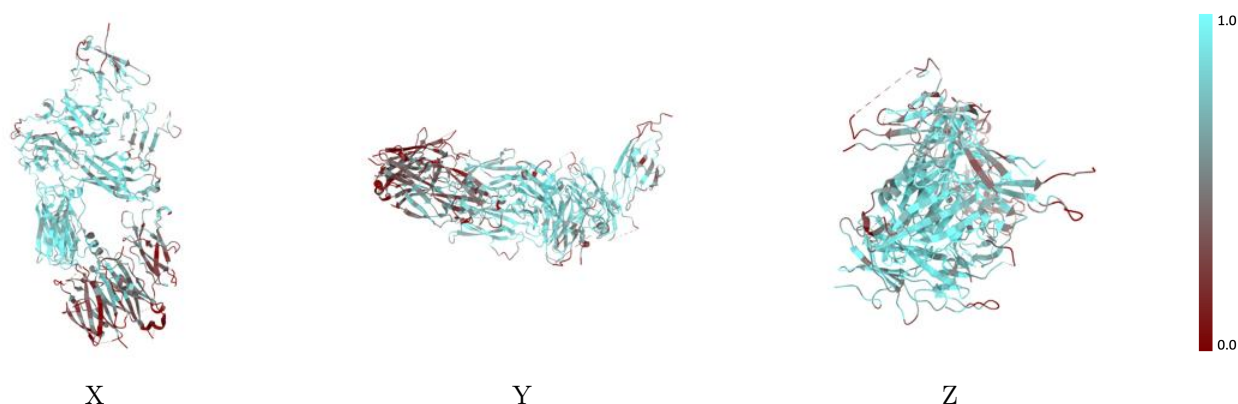
The images above show the 3D surface view of the map at the recommended contour level 0.249 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



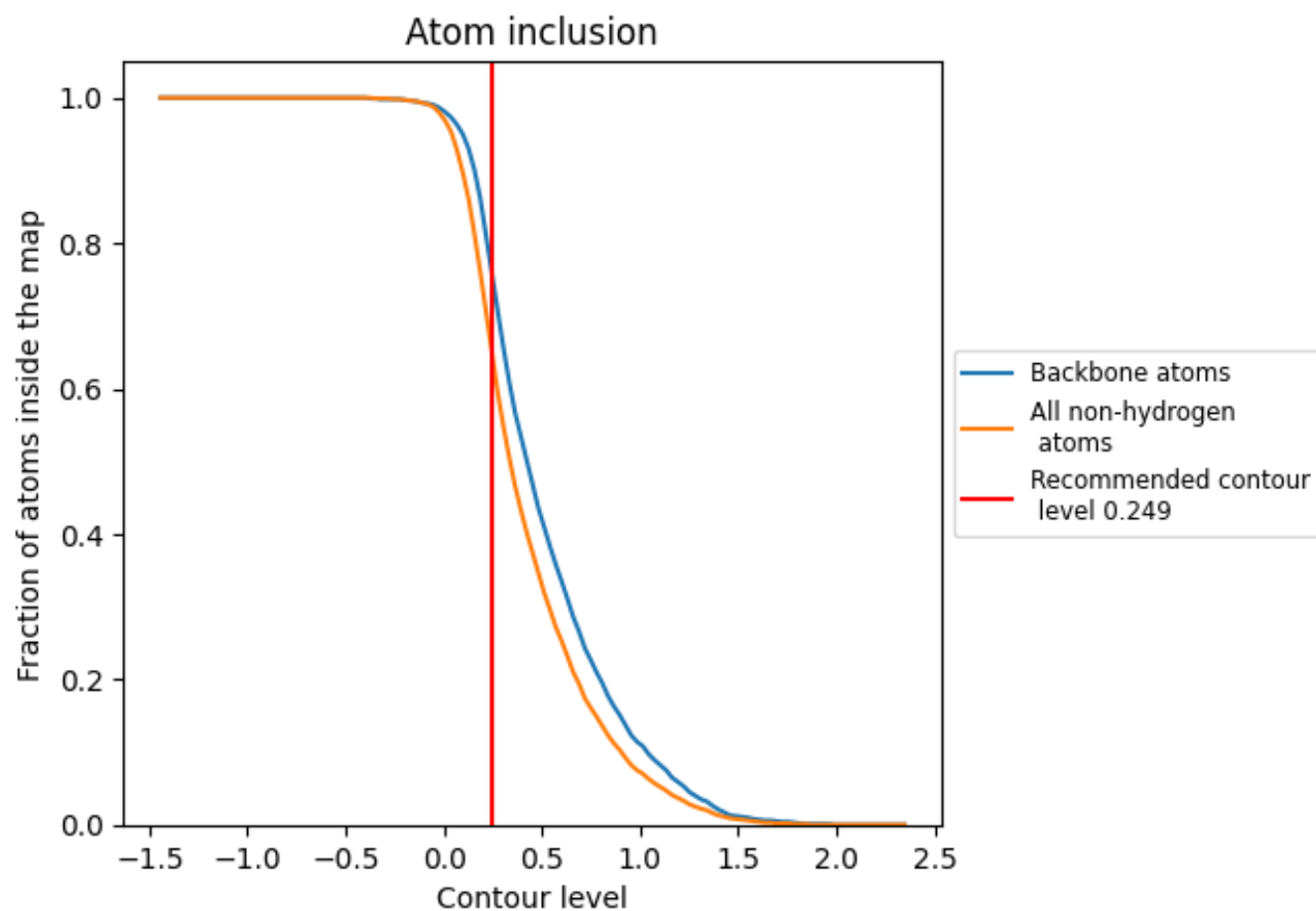
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.249).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.249) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6420	<div></div> 0.3780
A	<div></div> 0.6360	<div></div> 0.3290
B	<div></div> 0.5740	<div></div> 0.3670
C	<div></div> 0.7690	<div></div> 0.4230

